

# Contents of Volume 5

## COMMENTARIES

$\beta$ -Sheet rearrangements: serpins and beyond	J.A.Banzon and J.W.Kelly	113
---	--------------------------	-----

The structure of a protein bound to its receptor stimulates some new insights	P.R.Young	117
---	-----------	-----

Molecular surface area and hydrophobic effect	I.Tuñón, E.Silla and J.L.Pascual-Ahuir	715
---	--	-----

## PROTOCOLS

Efficient deletion mutagenesis by PCR	Z.B.Ogel and M.J.McPherson	467
---------------------------------------	----------------------------	-----

A novel sequential procedure to enhance the renaturation of recombinant protein from <i>Escherichia coli</i> inclusion bodies	B.Fischer, B.Perry, I.Sumner and P.Goodenough	593
---	---	-----

Recursive PCR: a novel technique for total gene synthesis	C.Prodromou and L.H.Pearl	827
---	---------------------------	-----

## PROTEIN STRUCTURE AND ANALYSIS

The crystal state binding of dithionite to deoxy-hemoglobin	F.C.Wireko and D.J.Abraham	3
---	----------------------------	---

Structure of a 16 kDa integral membrane protein that has identity to the putative proton channel of the vacuolar $H^+$ -ATPase	M.E.Finbow, E.E.Eliopoulos, P.J.Jackson, J.N.Keen, L.Meagher, P.Thompson, P.Jones and J.B.C.Findlay	7
--	---	---

Building protein backbones from $C\alpha$ coordinates	Y.Luo, X.Jiang, I.Lai, C.Qu, X.Xu and Y.Tang	147
---	--	-----

Quantitative analysis of protein far UV circular dichroism spectra by neural networks	G.Böhm, R.Muhr and R.Jaenicke	191
---	-------------------------------	-----

The $\alpha/\beta$ hydrolase fold	D.L.Ollis, E.Cheah, M.Cygler, B.Dijkstra, F.Frolow, S.M.Franken, M.Harel, S.J.Remington, I.Silman, J.Schrag, J.L.Sussman, K.H.G.Verschueren and A.Goldman	197
-----------------------------------	---	-----

The functions of tryptophan residues in membrane proteins	M.Schiffer, C.-H.Chang and F.J.Stevens	213
---	--	-----

Additional binding sites in lysozyme. X-ray analysis of lysozyme complexes with bromophenol red and bromophenol blue	Madhusudan and M.Vijayan	399
--	--------------------------	-----

Crystal structure of the high-alkaline serine protease PB92 from <i>Bacillus alcalophilus</i>	J.M.van der Laan, A.V.Tepljakov, H.Kelders, K.H.Kalk, O.Misset, L.J.S.M.Mulleners and B.W.Dijkstra	405
---	--	-----

The solution structure of echistatin: evidence for disulphide bond rearrangement in homologous snake toxins	R.M.Cooke, B.G.Carter, P.Murray-Rust, M.J.Hartshorn, P.Herzyk and R.E.Hubbard	473
---	---	-----

Site-directed mutagenesis and X-ray crystallography of two phospholipase $A_2$ mutants: Y52F and Y73F	M.M.G.M.Thunnissen, P.A.Franken, G.H.de Haas, J.Drenth, K.H.Kalk, H.M.Verheij and B.W.Dijkstra	597
---	--	-----

3-D structure of a mutant (Asp101→Ser) of <i>E.coli</i> alkaline phosphatase with higher catalytic activity	L.Chen, D.Neidhart, W.M.Kohlbrener, W.Mandecki, S.Bell, J.Sowadski and C.Abad-Zapatero	605
---	--	-----

<b>The structural consequences of exchanging tryptophan and tyrosine residues in <i>B.stearothermophilus</i> lactate dehydrogenase</b>	D.I.Roper, K.M.Moreton, D.B.Wigley and J.J.Holbrook	<b>611</b>
<b>Analysis of several key active site residues of ricin A chain by mutagenesis and X-ray crystallography</b>	Y.Kim and J.D.Robertus	<b>775</b>
<b>PREDICTION OF PROTEIN STRUCTURE</b>		
<b>Pattern-induced multi-sequence alignment (PIMA) algorithm employing secondary structure-dependent gap penalties for use in comparative protein modelling</b>	R.F.Smith and T.F.Smith	<b>35</b>
<b>A variable gap penalty function and feature weights for protein 3-D structure comparisons</b>	Z.-Y.Zhu, A.Sali and T.L.Blundell	<b>43</b>
<b>Evidence for a second conserved arginine residue in the integrase family of recombination proteins</b>	K.E.Abremski and R.H.Hoess	<b>87</b>
<b>A data bank merging related protein structures and sequences</b>	S.Pascarella and P.Argos	<b>121</b>
<b>Towards an automatic method of predicting protein structure by homology: an evaluation of suboptimal sequence alignments</b>	M.A.S.Saqi, P.A.Bates and M.J.E.Sternberg	<b>305</b>
<b>Computational complexity of a problem in molecular structure prediction</b>	J.T.Ngo and J.Marks	<b>313</b>
<b>Hydrophobicity and structural classes in proteins</b>	H.Cid, M.Bunster, M.Canales and F.Gazitúa	<b>373</b>
<b>IPSA—Inductive Protein Structure Analysis</b>	S.Schulze-Kremer and R.D.King	<b>377</b>
<b>Construction of a dictionary of sequence motifs that characterize groups of related proteins</b>	A.Ogiwara, I.Uchiyama, Y.Seto and M.Kanehisa	<b>479</b>
<b>Search for the stable state of a short chain in a molecular field</b>	A.V.Finkelstein and B.A.Reva	<b>617</b>
<b>A new approach to the design of a sequence with the highest affinity for a molecular surface</b>	B.A.Reva and A.V.Finkelstein	<b>625</b>
<b>Detection of secondary structure elements in proteins by hydrophobic cluster analysis</b>	S.Woodcock, J.-P.Mornon and B.Henrissat	<b>629</b>
<b>Potential of genetic algorithms in protein folding and protein engineering simulations</b>	T.Dandekar and P.Argos	<b>637</b>
<b>Protein secondary structure prediction using logic-based machine learning</b>	S.Muggleton, R.D.King and M.J.E.Sternberg	<b>647</b>
<b>Quantile distributions of amino acid usage in protein classes</b>	S.Karlin, B.E.Blaissdell and P.Bucher	<b>729</b>
<b>Relationships between sequence and structure for the four-<math>\alpha</math>-helix bundle tertiary motif in proteins</b>	C.D.Paliakasis and M.Kokkinidis	<b>739</b>
<b>MOLECULAR MODELLING AND DYNAMICS</b>		
<b>Molecular dynamics simulations of the whey protein <math>\beta</math>-lactoglobulin</b>	W.Gu and J.W.Brady	<b>17</b>
<b>Application of free energy simulations to the binding of a transition-state-analogue inhibitor to HIV protease</b>	A.Tropsha and J.Hermans	<b>29</b>
<b>Proline residues in transmembrane helices of channel and transport proteins: a molecular modelling study</b>	M.S.P.Sansom	<b>53</b>

Homology model of thyroxine binding globulin and elucidation of the thyroid hormone binding site	J.A.Jarvis, S.L.A.Munro and D.J.Craik	61
A robust and efficient automated docking algorithm for molecular recognition	N.Kasinos, G.A.Lilley, N.Subbarao and I.Haneef	69
A preliminary 3-D model of the tertiary fold of the polymerase domain of HIV-1 reverse transcriptase	L.S.Narasimhan and G.M.Maggiora	139
CD4 and CD8 may adopt a similar mode of binding to their MHC ligands	R.I.Brinkworth	151
Calculations of antibody-antigen interactions: microscopic and semi-microscopic evaluation of the free energies of binding of phosphorylcholine analogs to McPC603	F.S.Lee, Z.-T.Chu, M.B.Bolger and A.Warshel	215
An SS1-SS2 $\beta$ -barrel structure for the voltage-activated potassium channel	S.Bogusz, A.Boxer and D.D.Busath	285
Main structural and functional features of the basic cytosolic bovine 21 kDa protein delineated through Hydrophobic Cluster Analysis and molecular modelling	F.Schoentgen, N.Seddiqi, S.Bucquoy, P.Jollès, L.Lemesle-Varloot, K.Provost and J.-P.Mornon	295
Molecular modeling studies of the complex between cyclophilin and cyclosporin A	S.Gallion and D.Ringe	391
$\beta$ -sheet folding of fragment (16-36) of bovine pancreatic trypsin inhibitor as predicted by Monte Carlo simulated annealing	T.Nakazawa, H.Kawai, Y.Okamoto and M.Fukugita	495
Comparison of the modelled thyroxine binding site in TBG with the experimentally determined site in transthyretin	C.J.Terry and C.C.F.Blake	505
Molecular mechanics analysis of inhibitor binding to HIV-1 protease	C.E.Sansom, J.Wu and I.T.Weber	659
The T $\rightleftharpoons$ R structural transition of insulin; pathways suggested by targeted energy minimization	M.Engels, E.Jacoby, P.Krüger, J.Schlitter and A.Wollmer	669
Homology modeling of a heme protein, lignin peroxidase, from the crystal structure of cytochrome c peroxidase	P.Du, J.R.Collins and G.H.Loew	679
A molecular dynamics simulation of bacteriophage T4 lysozyme	G.E.Arnold and R.L.Ornstein	703
Hydration of amino acid side chains: dependence on secondary structure	A.S.Morris, N.Thanki and J.M.Goodfellow	717
The dimerization domain of LFB1/HNF1 related transcription factors: a hidden four helix bundle?	A.Pastore, R.De Francesco, M.A.Castiglione Morelli, D.Nalis and R.Cortese	749
Free energy perturbation study on a Trp-binding mutant (Ser <sup>88</sup> $\rightarrow$ Cys) of the <i>trp</i> -repressor	Y.Komeiji, M.Uebayasi, J.Someya and I.Yamato	759
<b>PROTEIN ENGINEERING</b>		
Biochemical properties of the kringle 2 and protease domains are maintained in the refolded t-PA deletion variant BM 06.022	U.Kohnert, R.Rudolph, J.H.Verheijen, E.J.D.Weening-Verhoeff, A.Stern, U.Opitz, U.Martin, H.Lill, H.Prinz, M.Lechner, G.-B.Kresse, P.Buckel and S.Fischer	93
Studies on chimeric fusion proteins of human aldolase isozymes A and B	Y.Takasaki and K.Hori	101

<b>Introduction of a stabilizing 10 residue <math>\beta</math>-hairpin in <i>Bacillus subtilis</i> neutral protease</b>	V.G.H.Eijsink, G.Vriend, B. van den Burg, J.R. van der Zee, O.R.Veltman, B.K.Stulp and G.Venema	<b>157</b>
<b>Increasing the thermostability of a neutral protease by replacing positively charged amino acids in the N-terminal turn of <math>\alpha</math>-helices</b>	V.G.H.Eijsink, G.Vriend, B. van den Burg, J.R. van der Zee and G.Venema	<b>165</b>
<b>Structure-activity relationships in human interleukin-1<math>\alpha</math>: identification of key residues for expression of biological activities</b>	H.Kawashima, J.-I.Yamagishi, M.Yamayoshi, M.Ohue, T.Fukui, H.Kotani and M.Yamada	<b>171</b>
<b>Site-directed mutagenesis of pseudoazurin from <i>Alcaligenes faecalis</i> S-6; Pro80Ala mutant exhibits marked increase in reduction potential</b>	M.Nishiyama, J.Suzuki, T.Ohnuki, H.Choon Chang, S.Horinouchi, S.Turley, E.T.Adman and T.Beppu	<b>177</b>
<b>Kinetic identification of a hydrogen bonding pair in the glucoamylase-maltose transition state complex</b>	M.R.Sierks and B.Svensson	<b>185</b>
<b>A functional antibody mutant with an insertion in the framework region 3 loop of the V<sub>H</sub> domain: implications for antibody engineering</b>	T.Simon and K.Rajewsky	<b>229</b>
<b>Phe496 and Leu497 are essential for receptor binding and cytotoxic action of the murine interleukin-4 receptor targeted fusion toxin DAB<sub>389</sub>-mIL-4</b>	F.Lakkis, B.Landgraf, Z.Wen, T.B.Strom and J.R.Murphy	<b>241</b>
<b>A point mutation that decreases the thermal stability of human interferon <math>\gamma</math></b>	C.A.Lunn, J.Fossetta, N.Murgolo, P.J.Zavodny, D.Lundell and S.K.Narula	<b>249</b>
<b>A point mutation of human interferon <math>\gamma</math> abolishes receptor recognition</b>	C.A.Lunn, J.Fossetta, D.Dalgarno, N.Murgolo, W.Windsor, P.J.Zavodny, S.K.Narula and D.Lundell	<b>253</b>
<b>Involvement of residues 296-299 in the enzymatic activity of tissue-type plasminogen activator</b>	N.F.Paoni, C.J.Refino, K.Brady, L.C.Peña, H.V.Nguyen, E.M.Kerr, A.C.Johnson, F.M.Wurm, R.van Reis, D.Botstein and W.F.Bennett	<b>259</b>
<b>A new protein conjugate that replaces the use of secondary antibodies engineered from the two staphylococcal enzymes protein A and 6-phospho-<math>\beta</math>-galactosidase</b>	E.Witt, G.C.Stewart and W.Hengstenberg	<b>267</b>
<b>Insertion of a disulfide-containing neurotoxin into <i>E.coli</i> alkaline phosphatase: the hybrid retains both biological activities</b>	D.Gillet, F.Ducancel, E.Pradel, M.Léonetti, A.Ménez and J.-C.Boulain	<b>273</b>
<b>Molecular modelling and site-directed mutagenesis on a bovine anti-testosterone monoclonal antibody</b>	T.Jackson, B.A.Morris, A.C.R.Martin, D.F.V.Lewis and P.G.Sanders	<b>343</b>
<b>Interchain cysteine bridges control entry of progesterone to the central cavity of the uteroglobin dimer</b>	W.Peter, R.Dunkel, P.F.W.Stouten, G.Vriend, M.Beato and G.Suske	<b>351</b>
<b>Protein engineering of the high-alkaline serine protease PB92 from <i>Bacillus alcalophilus</i>: functional and structural consequences of mutation at the S4 substrate binding pocket</b>	A.V.Tepliyakov, J.M.van der Laan, A.A.Lammers, H.Kelders, K.H.Kalk, O.Misset, L.J.S.M.Mulleners and B.W.Dijkstra	<b>413</b>
<b>The effect of cavity-filling mutations on the thermostability of <i>Bacillus stearothermophilus</i> neutral protease</b>	V.G.H.Eijsink, B.W.Dijkstra, G.Vriend, J.R.van der Zee, O.R.Veltman, B.van der Vinne, B.van den Burg, S.Kempe and G.Venema	<b>421</b>

Permuteins of interleukin 1 $\beta$ —a simplified approach for the construction of permuted proteins having new termini	R.A.Horlick, H.J.George, G.M.Cooke, R.J.Tritch, R.C.Newton, A.Dwivedi, M.Lischwe, F.R.Salemme, P.C.Weber and R.Horuk	427
Bipartite organization of the <i>Bacillus subtilis</i> endo- $\beta$ -1,4-glucanase revealed by C-terminal mutations	M.A.Hefford, K.Laderoute, G.E.Willick, M.Yaguchi and V.L.Seligy	433
Mutant forms of $\beta$ -galactosidase with an altered requirement for magnesium ions	I.S.Dunn and P.A.Jennings	441
Complex additivity of the effects of suppressor mutations in differing protein environments	I.S.Dunn and P.A.Jennings	447
Ligand requirements for Ca <sup>2+</sup> binding to EGF-like domains	M.Mayhew, P.Handford, M.Baron, A.G.D.Tse, I.D.Campbell and G.G.Brownlee	489
Effects of signal peptide changes on the secretion of bovine somatotropin (bST) from <i>Escherichia coli</i>	B.K.Klein, J.O.Polazzi, C.S.Devine, S.H.Rangwala and P.O.Olins	511
Improved insulin stability through amino acid substitution	D.N.Brems, P.L.Brown, C.Bryant, R.E.Chance, L.K.Green, H.B.Long, A.A.Miller, R.Millican, J.E.Shields and B.H.Frank	519
Altering the association properties of insulin by amino acid replacement	D.N.Brems, L.A.Alter, M.J.Beckage, R.E.Chance, R.D.DiMarchi, L.K.Green, H.B.Long, A.H.Pekar, J.E.Shields and B.H.Frank	527
Selection of a thermostable variant of chloramphenicol acetyltransferase (Cat-86)	S.L.Turner, G.C.Ford, A.Mountain and A.Moir	535
Cumulative stabilizing effects of glycine to alanine substitutions in <i>Bacillus subtilis</i> neutral protease	I.Margarit, S.Campagnoli, F.Frigerio, G.Grandi, V.De Filippis and A.Fontana	543
A structural role of histidine 15 in human glutathione transferase M1-1, an amino acid residue conserved in class Mu enzymes	M.Widersten and B.Mannervik	551
Analysis of disulphide bridge function in recombinant bovine prolactin using site-specific mutagenesis and renaturation under mild alkaline conditions: a crucial role for the central disulphide bridge in the mitogenic activity of the hormone	D.N.Luck, P.W.Gout, E.R.Sutherland, K.Fox, M.Huyer and M.Smith	559
Specificity determinants of rat tissue kallikrein probed by site-directed mutagenesis	J.Wang, J.Chao and L.Chao	569
Site-saturation mutagenesis and three-dimensional modelling of ROB-1 define a substrate binding role of Ser130 in class A $\beta$ -lactamases	J.-M.Juteau, E.Billings, J.R.Knox and R.C.Levesque	693
Single amino acid substitutions can further increase the stability of a thermophilic <i>L</i> -lactate dehydrogenase	H.K.W.Kallwass, W.K.Surewicz, W.Parris, E.L.A.Macfarlane, M.A.Luyten, C.M.Kay, M.Gold and J.B.Jones	769
Triple point mutation Asp10 $\rightarrow$ His, Asn101 $\rightarrow$ Asp, Arg148 $\rightarrow$ Ser in T4 phage lysozyme leads to the molten globule	V.N.Uversky, V.V.Leontiev and A.T.Gudkov	781
Probing the role of threonine and serine residues of <i>E.coli</i> asparaginase II by site-specific mutagenesis	C.Derst, J.Henseling and K.H.Röhm	785
Construction and characterization of a single polypeptide chain containing two enzymatically active dihydrofolate reductase domains	M.Iwakura and C.R.Matthews	791



## CLONING EXPRESSION

- Overproduction, preparation of monoclonal antibodies and purification of *E.coli* asparagine synthetase A** S.K.Hinchman and S.M.Schuster 279
- Active papain renatured and processed from insoluble recombinant propapain expressed in *Escherichia coli*** M.A.J.Taylor, K.A.Pratt, D.F.Revell, K.C.Baker, I.G.Sumner and P.W.Goodenough 455
- Over-production of 5-enolpyruvylshikimate-3-phosphate synthase in *Escherichia coli*: use of the T7 promoter** W.A.Shuttleworth, C.D.Hough, K.P.Bertrand and J.N.S.Evans 461
- Expression of the phosphorylase kinase  $\gamma$  subunit catalytic domain in *Escherichia coli*** S.Cox and L.N.Johnson 811

## PHYSICO-CHEMICAL STUDIES OF PROTEIN STRUCTURE AND FUNCTION

- Fluorescent properties of the *Escherichia coli* D-xylose isomerase active site** A.C.Jamieson and C.A.Batt 235
- pH-sensitive interactions between IgG and a mutated IgG-binding protein based upon two B domains of Protein A from *Staphylococcus aureus*** M.G.Gore, W.F.Ferris, A.G.Popplewell, M.Scawen and T.Atkinson 577
- Oxygen binding and other physical properties of human hemoglobin made in yeast** K.Adachi, P.Konitzer, C.H.Lai, J.Kim and S.Surrey 807

## SYNTHETIC GENES AND PROTEINS

- Expression of a synthetic gene coding for the amino acid sequence of *Clostridium pasteurianum* rubredoxin** M.K.Eidsness, S.E.O'Dell, D.M.Kurtz,Jr, R.L.Robson and R.A.Scott 367
- Overexpression and structure-function analysis of a bioengineered IL-2/IL-6 chimeric lymphokine** F.Rock, M.Everett and M.Klein 583
- Computer-aided gene design** G.Libertini and A.Di Donato 821

## PROTEIN AND PEPTIDE CHEMISTRY

- Characterization of the interactions of a bifunctional inhibitor with  $\alpha$ -thrombin by molecular modelling and peptide synthesis** S.-Y.Yue, J.DiMaio, Z.Szewczuk, E.O.Purisima, F.Ni and Y.Konishi 77
- Uncoupling of catalysis and colipase binding in pancreatic lipase by limited proteolysis** A.Abousalham, C.Chaillan, B.Kerfelec, E.Foglizzo and C.Chapus 105
- Design, synthesis and structure of an amphipathic peptide with pH-inducible haemolytic activity** R.Moser 323
- Nuclear magnetic resonance studies and molecular dynamics simulations of the solution conformation of a 'designed',  $\alpha$ -helical peptide** W.Klaus and R.Moser 333
- Cellulose-binding domains: potential for purification of complex proteins** J.M.Greenwood, E.Ong, N.R.Gilkes, R.A.J.Warren, R.C.Miller,Jr and D.G.Kilburn 361
- Development of an optimized refolding process for recombinant Ala-Glu-IGF-1** K.R.Hejnaes, S.Bayne, L.Nørskov, H.H.Sørensen, J.Thomsen, L.Schäffer, A.Wollmer and L.Skriver 797

